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Vibrational properties and magnetic specific heat of the covalent chain antiferromagnet RbFeS e2

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Abstract

© 2018 American Physical Society. The magnetic specific heat of RbFeSe2 and the spin state of Fe3+ ions in the compound have been studied. Phonon dispersion and phonon density of states (PDOS), element specific and total, were evaluated from first-principles calculations. It is shown that iron atoms in quasi-one-dimensional chains have dramatically different vibrational properties against Rb and Se atoms: the Fe PDOS is mostly concentrated within two Einstein-like optical phonon peaks at high frequencies. Analysis of our Mössbauer data for RbFeSe2, utilizing the calculated Fe PDOS as well as our optical absorption measurements, have shown full agreement with the location of the high-frequency optical-type lattice vibrations within the FeSe4 tetrahedra. The calculated PDOS was utilized to evaluate the lattice contribution to the specific heat. The phonon heat capacity has been used to evaluate the magnetic specific heat of the quasi-one-dimensional antiferromagnetically correlated Fe3+ ion chains in RbFeSe2. An intermediate spin state S=3/2 has been found most closely relevant to our magnetic entropy analysis for Fe3+ ions in RbFeSe2.

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